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Diffractive–refractive optics in the Laue case: first experiment

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The possibility of sagittally focusing synchrotron radiation using an asymmetric Laue crystal with profiled surfaces has been experimentally demonstrated for the first time. The sample was a Si single crystal with two parallel cylindrical holes of diameter 8 mm. The axes of the holes formed an angle of 7.95° with the (111) diffracting planes and were arranged vertically with respect to the diffracting planes. 15.35 keV synchrotron radiation was diffracted in the space between the holes. The minimum thickness of this Laue crystal was 0.5 mm. The diffracted beam formed an angle of 0.55° with the exit surface. The experiment was performed at beamline BM05 at the ESRF. The length of the beamline was not sufficiently long to detect the focus, but the experiment clearly showed that the diffracted beam was sagittally convergent.

Keywords: asymmetric Laue diffraction; sagittal focusing; diffractive–refractive optics; sagittally focusing Laue crystal; X-ray monochromator.

1. Introduction

If an X-ray beam is impinging on a crystal surface which is inclined with respect to the diffracting crystallographic planes, then the diffracted beam is slightly deviated from that which would be diffracted from a surface parallel to the diffracting planes. If the inclination is such that the normal to the surface and the normal to the diffracting planes form a plane which is perpendicular to the plane of diffraction (the plane determined by the normal to the diffracting planes and the impinging beam), then the beam is deviated sagittally. Let us call this kind of surface inclination sagittal inclination. In Bragg-case diffraction this effect has already been studied in detail by Hrdý (2001, and the references therein). It was shown that this effect may be utilized to sagittally focus the diffracted radiation if the diffraction surface is profiled into a longitudinal parabolic shape. This has been proved experimentally at ESRF, APS and NSLS (Hrdý & Siddons, 1999; Artemiev *et al.*, 2001, 2003; Hrdý *et al.*, 2001). This kind of optics is called Bragg diffractive–refractive optics, because the effect of the sagittal deviation of the diffracted beam is due to refraction occurring during Bragg diffraction. To our knowledge this kind of optics has not been installed anywhere so far. This is another way of utilizing refraction for focusing contrary to well known X-ray refraction lenses (Snigirev *et al.*, 1996).

Recently, the sagittal deviation of the diffracted beam from a sagittally inclined surface was studied for Laue-case asymmetric diffraction (Hrdý, Hoszowska & Mocella, 2003). In this work the sagittal deviation of the diffracted beam from a flat asymmetric Laue crystal with sagittally inclined wedge was observed experimentally. Unfortunately the image presented in this paper did not allow easy and straightforward observation of the sagittal shift. For this reason the experiment was repeated at the ESRF (Hrdý, Hoszowska, Mocuta *et al.*, 2003) under the same conditions, except that the thickness of the Si Laue crystal was reduced to 0.25 mm (Fig. 1). Fig. 1 shows clearly the separation of the beam which was diffracted from the wedge. [Diffraction occurred on the (111) planes which formed an angle of 10.7° with the surface, and the wavelength was 0.1 nm.] The simple theory presented by Hrdý, Hoszowska & Mocella (2003) gives the formula for the sagittal deviation δ of the beam diffracted from a sagittally inclined surface,

$$\delta = (PN/k)\tan\beta = \{Lp[\cos\theta/\cos(\theta+\alpha)]/k\}\tan\beta, \qquad (1)$$

where

$$Lp = \big[r_{\rm e}\lambda/(2\pi V\cos\theta_{\rm B})\big]\big[F_{0{\rm r}} - \rho|F_{h{\rm r}}|\exp(-M)\big]. \qquad (2)$$

Here $r_{\rm e}$ is the classical electron radius, V is the volume of the unit cell, $\theta_{\rm B}$ is the Bragg angle, ρ is the polarization factor, $F_{0{\rm r}}$ and $F_{h{\rm r}}$ are the real parts of the structure factors of the corresponding reflections (see, for example, Batterman & Cole, 1964) and $k = 1/\lambda$. The angle α is the deviation of the entrance surface from that in the Laue symmetrical case and β is the inclination angle. Here it is assumed that in the vicinity of the Laue point the Ewald spheres may be replaced by planes.

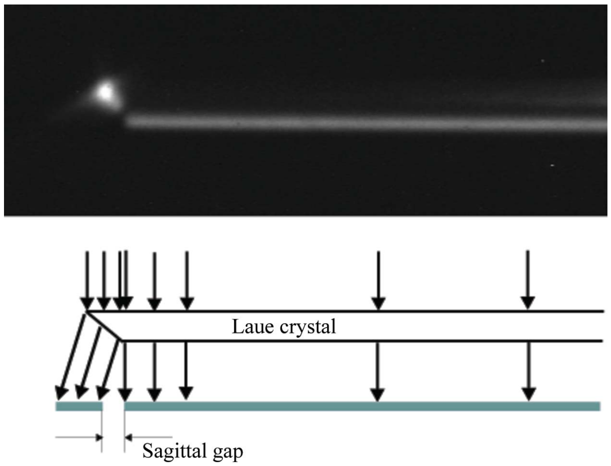

Figure 1
Image of the beam diffracted from the Laue crystal with the wedge produced in the lateral part of the crystal. The beam diffracted on the wedge is deviated both sagittally and meridionally. A schematic diagram of the diffraction is shown in the lower part of the picture. The width of the wedge was 0.14 mm.

As was suggested by Hrdý, Hoszowska & Mocella (2003), the above-discussed effect of sagittal deviation may be utilized to sagittally focus synchrotron radiation using a Laue crystal with a longitudinal parabolic profile of one or both diffracting surfaces. Equation (1) is analogous to the formula (7),

$$\delta = K \tan \beta, \quad (3)$$

taken from Hrdý (1998) where for silicon $K = (1.256 \times 10^{-3}) d_{hkl}$ [nm] λ [nm]. As was shown there, this leads directly to a longitudinal parabolic shape for the diffracting surface. The parabola is described by the equation

$$y = ax^2, \quad (4)$$

where

$$a = (S + f)/(2NKfS). \quad (5)$$

Here S is the crystal–source distance, f is the focal distance of the crystal, and N is the number of diffraction events. The parabolic surface may be approximated by a circular hole of diameter D, where $D = 1/a$. Obviously (4) and (5) could be applied to the design of a sagittally focusing Laue crystal with profiled diffracting surface (parabolic or circular) if K is replaced by $Lp[\cos\theta/\cos(\theta + \alpha)]/k$. This is valid if only the exit surface is profiled and for the diffracted (not forward-diffracted) beam (see Fig. 2). The entrance surface influences the sagittal direction of the diffracted beam much less. The distance PN in (1) should be replaced by

$$PR = Lp[\cos\theta/\cos(\alpha - \theta)]. \quad (6)$$

(To understand the meaning of distances PR and Lp in reciprocal space, see Hrdý, Hoszowska & Mocella, 2003.)

Sagittal focusing of synchrotron radiation is normally achieved by sagittal bending of the second crystal of a Bragg crystal monochromator (Sparks *et al.*, 1982). Bragg diffractive–refractive optics is the alternative method, which may be advantageous for long focusing distances and not too broad a

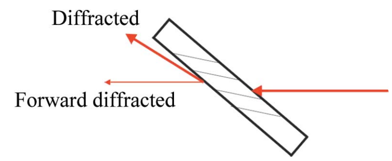

Figure 2
The Laue-diffracted beam is split into two beams: diffracted and forward-diffracted beams.

range of wavelengths. (This is because the sagittal deviation is not too sensitive to sagittal tilt. For this reason, creating a focus of a synchrotron radiation beam at a long distance does not require very high precision in the realisation of a focusing element, as is for example the case of mirrors or bent crystals.) Also, sagittal focusing by a Laue monochromator may be realised by sagittal bending, but only if the crystal is asymmetrical (Zhong *et al.*, 2001*a*,*b*).

In this paper we will demonstrate experimentally the possibility of sagittal focusing of X-ray synchrotron radiation by a Laue crystal with profiled diffracting surfaces.

2. Experiment

For the experiment we used an asymmetrical Si Laue crystal, shown in Figs. 3 and 4. The diffracting part is the space between two longitudinal cylindrical holes with diameter $D = 1/a = 8$ mm. (The circle with diameter $D = 1/a$ is a good approximation of parabola $y = ax^2$ for small x.) The walls of the holes represent sagittal tilt. The (111) diffracting crystallographic planes are deviated from the entrance surface by 7.95°, so that $\alpha = 82.05°$. Both the entrance and exit diffraction surfaces were mechano-chemically polished. The experiment was performed at beamline BM05 at the ESRF (MI751).

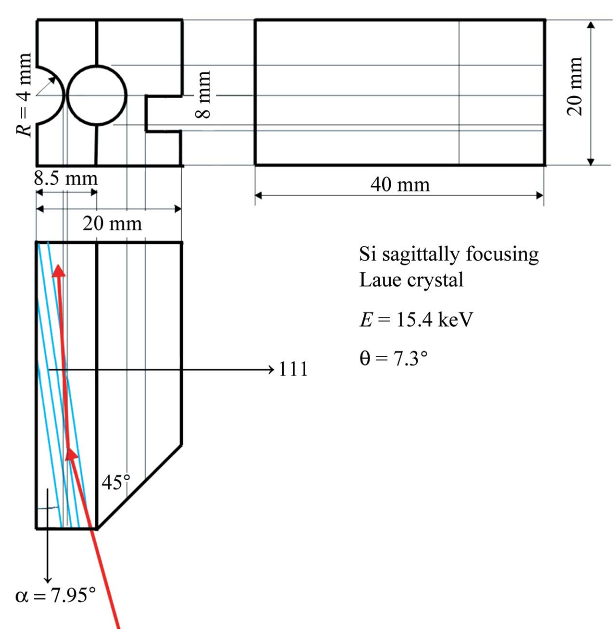

Figure 3
Drawing of the Laue crystal.

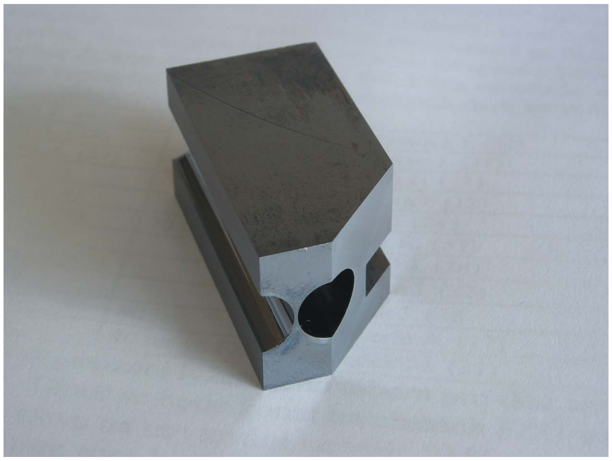

Figure 4
Photograph of the Laue crystal.

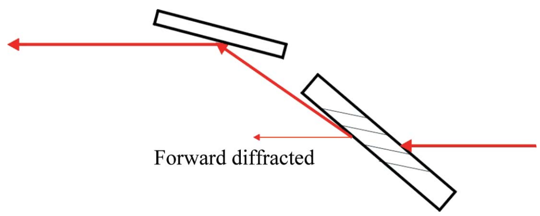

Figure 5
Arrangement of the experiment. The Laue-diffracted beam is further diffracted from a Bragg symmetric crystal to redirect the diffracted beam into the horizontal direction.

The experimental arrangement is shown in Fig. 5. To limit the presence of harmonics in the beam and to avoid the problem with energy determination, we used a primary monochromator which was set to 15.35 keV ($\theta = 7.4^\circ$) and was de-tuned. There are two beams which were diffracted from the crystal. The forward-diffracted beam was not used, because the refraction effect is small (the refraction effect is stronger for beams forming a smaller angle with a surface). The diffracted beam which was used formed an angle of 0.55° with the crystal exit surface and was deviated from the horizontal plane by an angle $2\theta = 14.8^\circ$. To redirect this diffracted beam into the horizontal direction a (111) Bragg crystal was placed after the Laue crystal. Even if we had used a white beam this combination of the Laue and Bragg crystals would have allowed us to reject higher harmonics. (The angular distributions of harmonics for Bragg and Laue diffraction are different.) The beam size was delimited by a 3 mm × 3 mm slit located before the Laue crystal. The crystals–source distance was 35 m.

For the above arrangement, $Lp[\cos\theta/\cos(\theta+\alpha)]/k$ = 9.956×10^{-5} ($F_0 = 112$, $F_{111,r} = 59.7$, $V = 0.15994$ nm^3, $r_e = 2.818 \times 10^{-6}$ nm, $d_{111} = 0.313397$ nm). Substituting this value into (5), the focusing distance for $N = 1$ is −272 m. [Note the sign (−) which means that the beam is still divergent.] This is the focusing distance created only by the exit surface. The additional effect of the entrance surface may be calculated according to the recurrent formula of Hrdý *et al.* (2005). {Another possibility is simply to replace K in (5) by $Lp(\cos\theta/\cos(\theta+\alpha) + Lp[\cos\theta/\cos(\alpha-\theta)]$.} The calculation gives a focusing distance of −360 m. Practically, the Laue crystal should transfer the sagittally divergent beam into an almost parallel beam.

To check this behavior we put an X-ray film and a CCD detector 20 m downstream from the crystal (a longer distance was not available) and recorded the image together with the image taken just after the crystals.

3. Results

Fig. 6(*a*) shows an image of the diffracted beam at a small distance after the Bragg crystal. The horizontal (sagittal) dimension of the spot, *i.e.* the distance between the border beams A and B, is 3.22 mm. The shape of the spot is a narrow 'smile' because of the circular profile of the diffracting surfaces and the asymmetric diffraction. The image taken at 20 m from the crystal (Fig. 6*b*) is more complicated, having the shape of a horse-shoe. The border beams A and B are sagittally deviated such that their distance is 1.72 mm. Without focusing, the distance between both beams would be 3.22 × (55/35) = 5 mm (the crystals–source distance is 35 m and the detector–source distance is 55 m). Together with the sagittal deviation, the beams are also sagittally spread (see the dimensions a and b). The above theory was developed for the beams at the center of the diffraction region, *i.e.* only point P on the diffraction surface was considered (Hrdý, Hoszowska, Mocuta *et al.*, 2003). Considering the whole part of the dispersion surface where the diffraction intensity is significant results in the sagittal spread. This situation is analogous to the Bragg diffractive–refractive optics if only one crystal is used. The higher the deviation, the higher the spread. The conse-

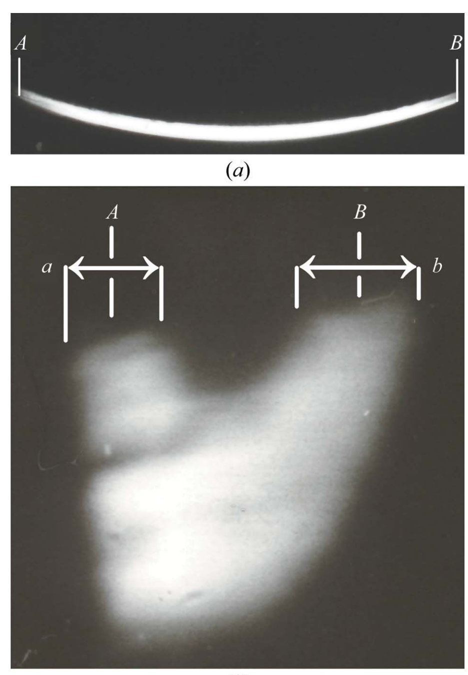

Figure 6
(*a*) Image of the beam taken just after the Bragg crystal. The image taken 20 m from the Bragg crystal (*b*) shows the sagittal squeezing of the beam. The distance AB in (*a*) is 3.22 mm, whereas in (*b*) it is 1.72 mm.

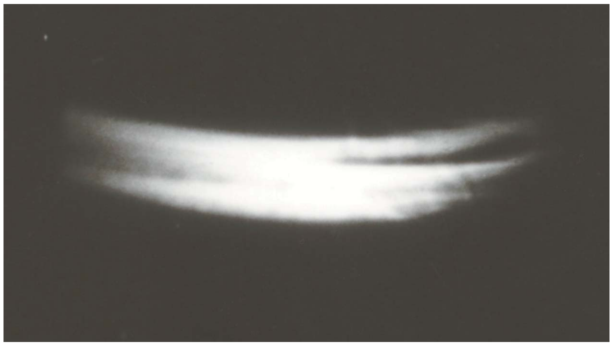

Figure 7
Image of the beam taken 7 m from the crystals, showing the meridional splitting of the diffracted beam (partially seen also in Fig. 6*b*).

quence of this is that one crystal, or more crystals in non-dispersive arrangement, cannot give a sharp focus. Only two or more crystals in dispersive arrangements completely cancel the sagittal spread so that the focus may be sharp (Hrdý & Siddons, 1999). We suppose that the same holds for the Laue diffractive–refractive optics.

From the distances between the beams *A* and *B* near the crystals and at 20 m from the crystals we can deduce that the focusing distance is about +43 m, contrary to the theoretical prediction.

Fig. 7 shows an image taken at about 7 m from the crystals. It is interesting to note that the beam seems to be vertically split into two or even three beams. This may also be seen in Fig. 6(*b*).

Owing to highly asymmetric diffraction the beam diffracted from the Laue crystal has a relatively large vertical divergence, which explains the large vertical size of the spot at 20 m from the crystal (about 2.4 mm). This somewhat devaluates the intensity gain due to the sagittal concentration of the beam. Here the vertical size of the beam at 43 m from the crystal would be $2.4 \times (43/20) = 5.16$ mm. Without the Laue crystal, the vertical size of the beam at 43 m would be $3 \times (78/35) = 6.7$ mm ($78 = 35 + 43$).

4. Discussion

The above-described experiment shows that the idea of diffractive–refractive optics developed for Bragg-case diffraction in the past can be also extended to Laue-case diffraction. It was shown that the asymmetric Laue crystal with profiled diffracting surfaces may concentrate the diffracted beam and thus increase the intensity in the diffraction spot. The calculation predicted an almost parallel diffracted beam in the sagittal direction but the experiment showed a convergent beam with estimated focus at 43 m. As the diffraction was highly asymmetric, the focusing distance is very sensitive to $\cos\theta/\cos(\theta+\alpha)$, where $\theta+\alpha$ is close to 90°. A small uncertainty in the knowledge of α and β may substantially influence the focusing distance calculation. This may be an explanation of the discrepancy between the experiment and calculation. Obviously, further theoretical and experimental work is needed.

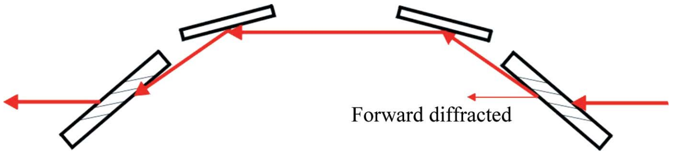

Figure 8
Schematic picture of the four-crystal dispersive arrangement. The Laue crystals have profiled diffracting surfaces.

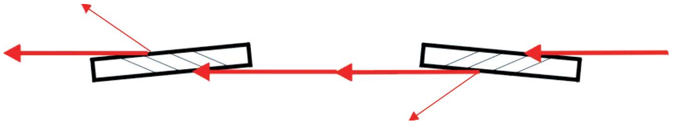

Figure 9
Schematic picture of two Laue crystals with profiled diffracting surfaces arranged in dispersive position.

As mentioned above, owing to the sagittal spread the focus cannot be sharp. The distribution of the intensity at the focal spot could not be studied experimentally because the beamline was not long enough. Obviously this type of focusing device is suitable only for long focusing distances and narrow wavelength tunability range.

To improve the quality of the focus, *i.e.* to cancel the sagittal and vertical spreads, two Laue crystals with profiled surfaces in dispersive setting should be used (see the analogy with Bragg diffractive–refractive optics). There are two possibilities. The first one is shown in Fig. 8. This arrangement should give a shorter focusing distance and should allow for the harmonics rejection, but is rather complicated. The arrangement shown in Fig. 9 should give the shortest focusing distance, because both entrance and exit diffracting surfaces create equal sagittal deviation of the beam. For calculation of the focusing distance, equation (5) may be used, taking $N = 4$. This gives a focusing distance of about 14 m. The drawback is that in highly asymmetric diffraction the vertical size of the beam must be small or the crystals size must be large.

The use of the additional Laue crystal means an additional decrease of diffracted intensity because of the splitting of the diffracted beam.

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